CompassCDS
Arithmetic Functions Plug-in
User Guide

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2017
Publication Number BR501487
Revision D

Contents

Software Presentation....3
Overview....3
Installation....3
Application Details....4
How to Use the Arithmetic Functions Plug-in....4
Operand Selection....5
Operator Selection....6
Calculation Parameters....7
Addition....7
Subtraction....8
Multiplication....8
Division....8
Weighting Sum....8
Generation of a Chromatogram Usable in CompassCDS....10
Saving the Generated Chromatogram....10
Loading a Virtual Chromatogram in CompassCDS....10
Returning to CompassCDS without Generating a Virtual Chromatogram....11

Software Presentation

This document describes the Arithmetic functions Plug-in for CompassCDS.

Overview

The Arithmetic functions Plug-in enables mathematical operations between either chromatograms or chromatograms and real numbers.

It operates like a calculator with two operands, one operator and one result.

Each operand can be either selected among chromatograms loaded in CompassCDS or in the chromatograms storage directory. A numerical zone is also available to execute an operation between a chromatogram and a real number.

Different operators are available and these include: Addition, Multiplication, Subtraction, Division, and Weighted sum.

Once the operands have been selected, the operation is validated by clicking on the operator button. The result is then displayed in the bottom left of the screen.

Installation

Insert the CompassCDS media in the CD/DVD drive.

Check the following files are present in the C:\CompassCDS\client folder.

- AX_arithmetic.dll
- Diamirdefaultmethod.meth: It allows the user to save calculated chromatograms with this default CompassCDS method

Select the AX_Arithmetic.dll file and drag and drop it on the C:\CompassCDS\client \TRegSvr.exe to merge the file with the registry.

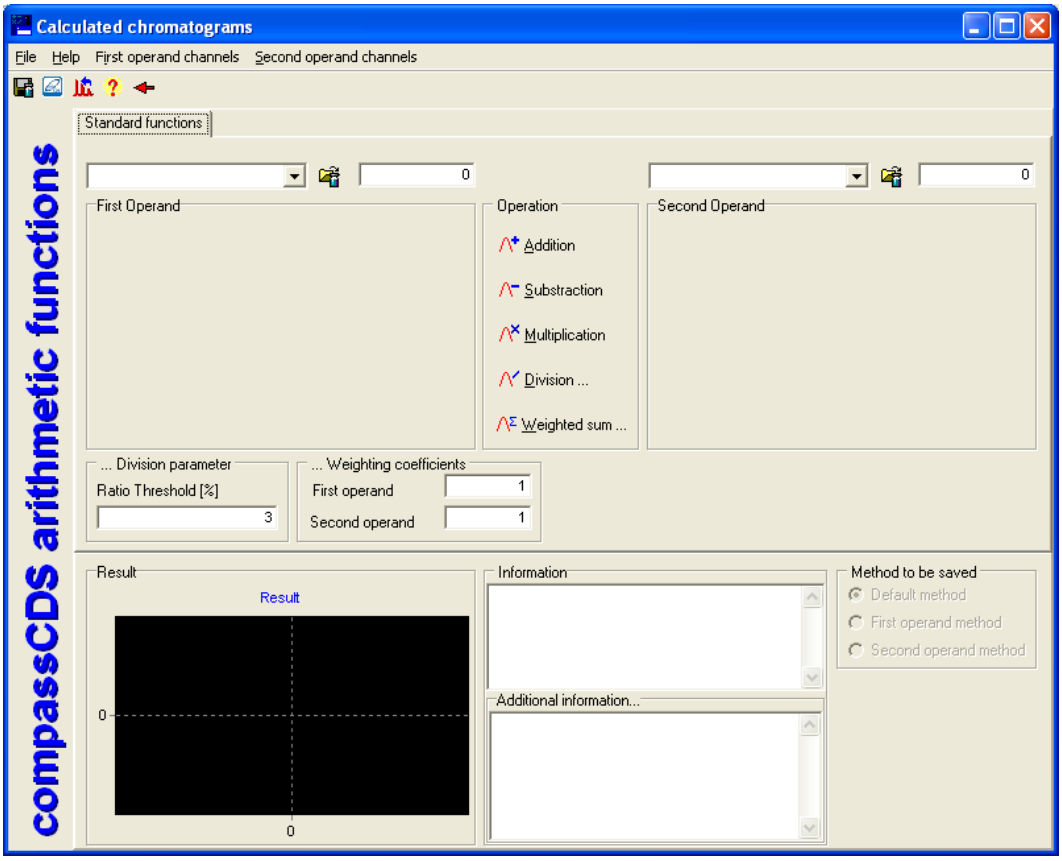
Start CompassCDS, check that the icon allows to access the “Arithmetic functions” plug-in.

Application Details

How to Use the Arithmetic Functions Plug-in

In CompassCDS, open the Arithmetic plug-in by selecting the

icon. The following screen is displayed:



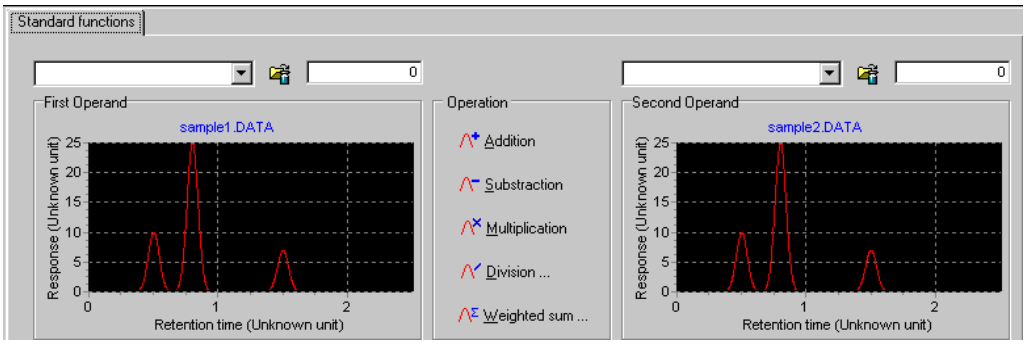
The main screen is divided into two parts:

The first part enables a user to select the chromatogram(s) on which the calculations (called Operand) is performed, and the type of calculation (by choosing Operation) which will define the function. A second part is dedicated to result viewing.

Icons enable a user to save the virtual chromatogram generated, and open it into the current CompassCDS session.

Operand Selection

The two operands are located in the top left and right of the screen. The operand can be a chromatogram or a real number.

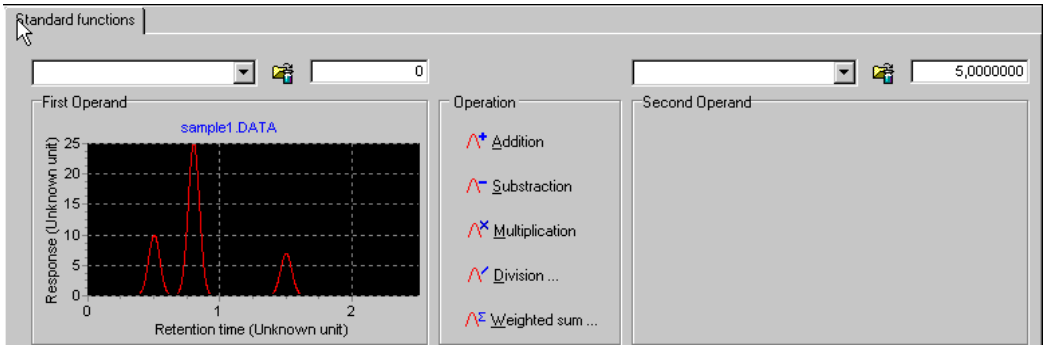


To select Chromatograms, a user has two options:

- If the chromatogram is open in the CompassCDS session, select its name from the scrolling list: .
- If the chromatogram is not open in the CompassCDS session, select the chromatogram via the button.

In an operation between a real number and a chromatogram, the numerical zone next to chromatogram names must be completed. Only one chromatogram and one real number can be entered. The chromatogram is defined in one operand part (left or right) and the real number in the other.

The following screen is displayed:



Operator Selection

Once two operands (2 chromatograms or 1 chromatogram and a real number) have been defined, the user can select the desired operator.

Five operators are available:

Addition

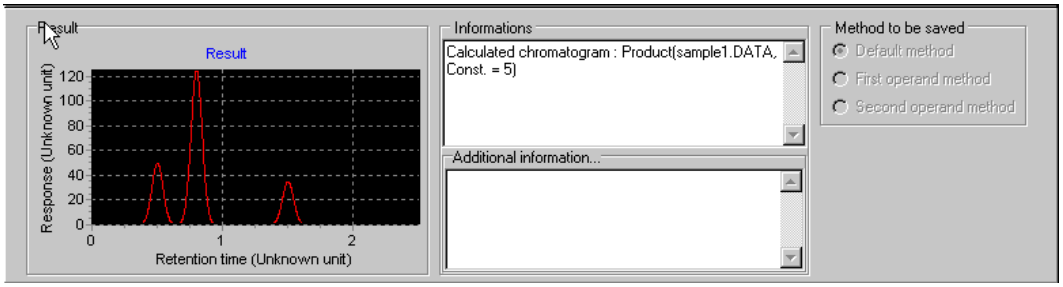
Subtraction

Multiplication

Division

Weighted Sum

As soon as the operator is selected, the result is displayed in the Result part of the screen:



NOTE: The sampling interval and delay time must be identical to process the calculation between chromatograms.

If the retention unit or the response unit is different between chromatograms, a warning is displayed and a user must choose to either ignore the problem and process the calculation, or to cancel it.

If the units are different, the unit saved in the result chromatogram is “Different unit”. If the units are unknown in all the chromatogram parameters, “Unknown unit” will be saved.

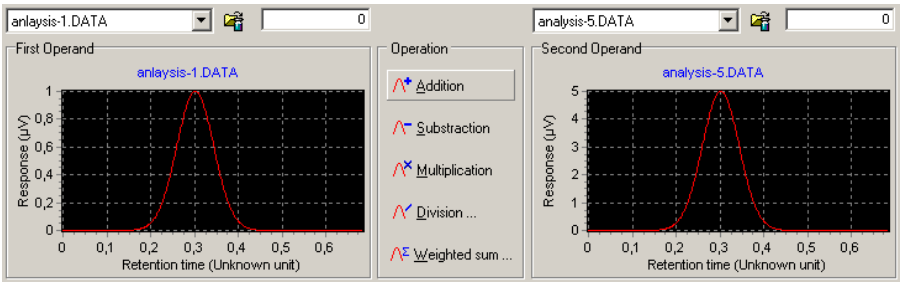
NOTE: If a multi-channel chromatogram is loaded into the Arithmetic Functions Plug-in, a user must select the channel on which calculations are to be performed in the FIRST OPERAND CHANNELS or the SECOND OPERAND CHANNELS menus.

Calculation Parameters

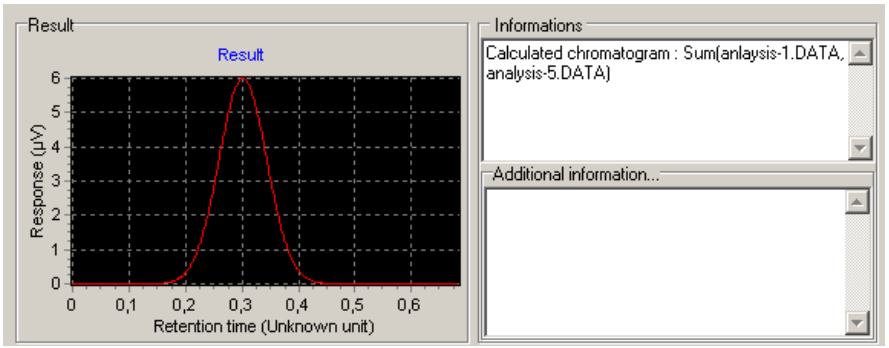
Addition

Two chromatogram plots can be added by selecting two chromatograms as operands, or add a value to all points of the chromatogram plot, then activate the Addition operator.

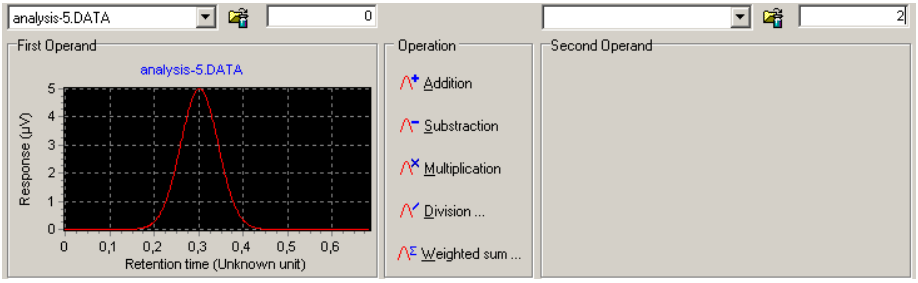
Chromatogram and Operator Selection: Two chromatograms



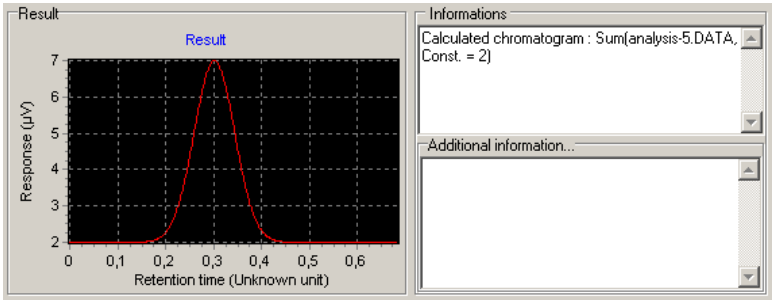
Result:



Chromatogram and Operator Selection: One Chromatogram and One Operator



Result:



Subtraction

Subtract one chromatogram from another chromatogram by selecting two chromatograms as operands, or subtract a value from all points of the chromatogram plot. Then the subtraction is performed by activating the operator.

NOTE: In case of subtraction of two chromatograms, the second one (second operand) is subtracted from the first one (first operand).

Multiplication

Multiply one chromatogram by another chromatogram by selecting two chromatograms as operands, or multiply all points of the chromatogram. The multiplication is performed by activating the

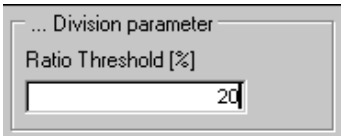
operator. If two chromatograms are multiplied, the signal value is multiplied point by point.

Division

Divide one chromatogram by another chromatogram by selecting two chromatograms as operands, or divide all points of the chromatogram. The division is performed by activating the

operator.

The ratio threshold % must be defined. The ratio chromatogram threshold determines a maximum value for ratio calculation when performing the “Division” function.



When performing the A/B division, if the signal intensity of the first chromatogram (A) multiplied by the ratio chromatogram threshold (in %) and divided by 100, is superior to the signal intensity of the second chromatogram (B), then the ratio is set to 0.

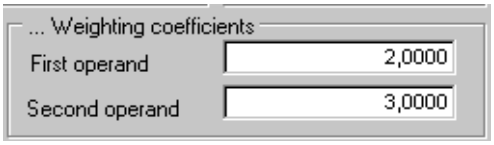
For example, if the ratio threshold is set to 20%, the ratio will be set to 0 if B<0.2A

This means that the intensity of the second chromatogram represents too small a percentage of the first chromatogram. So, the ratio chromatogram threshold sets the percentage of rejection.

Weighting Sum

This operation allows users to perform weighting addition operands. For example (2*First operand) + (3*Second operand).

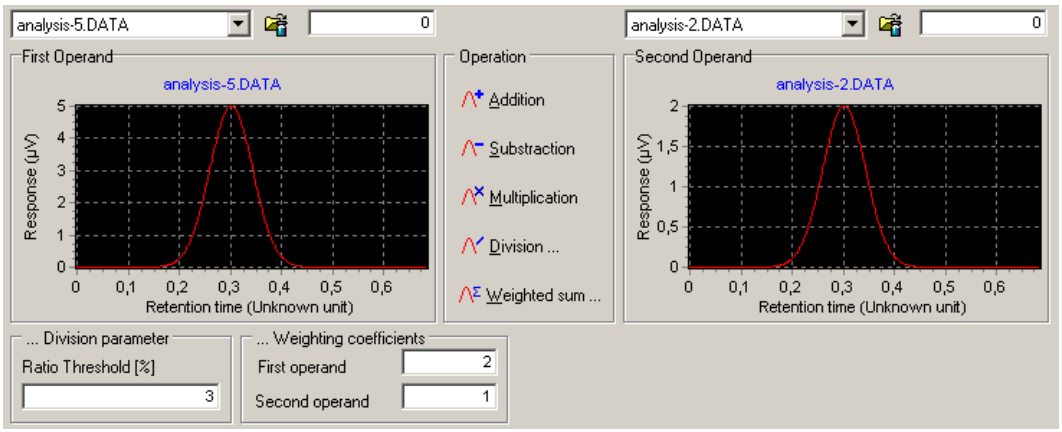
A user enters the first and second weighting coefficients, respectively for the first and second operand. These will be used to perform the sum.



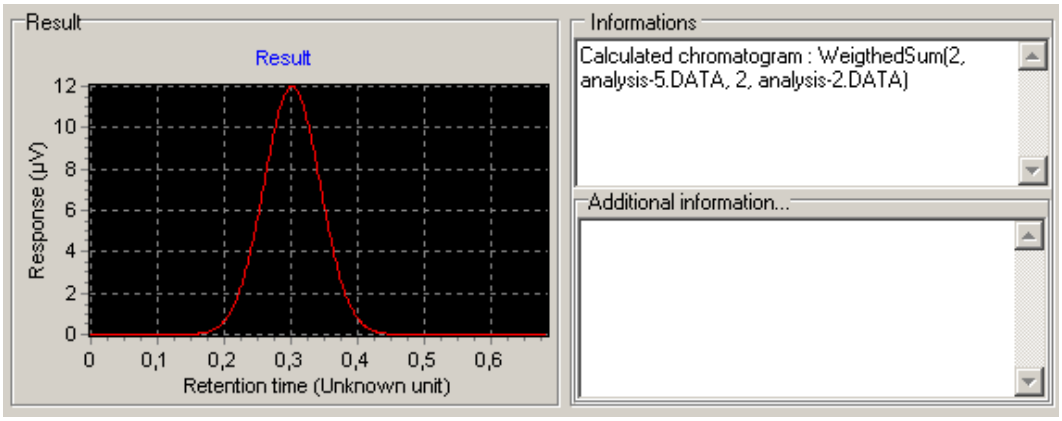
The

operator is then activated

Chromatogram and Operator Selection: Two Chromatograms with Weighting Coefficients.



Result:



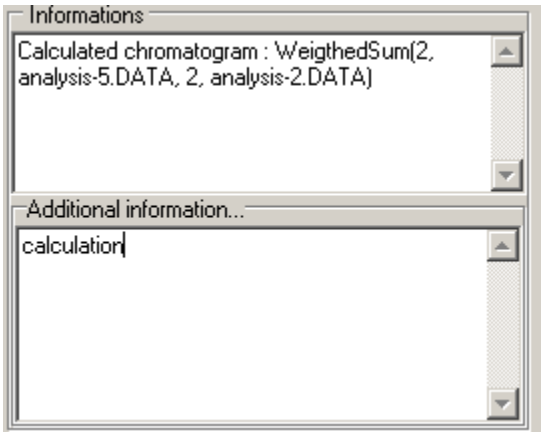
Generation of a Chromatogram Usable in CompassCDS

Saving the Generated Chromatogram

The virtual chromatogram generated can be saved as a .VIRT file. Then, it can be processed as a normal chromatogram in CompassCDS.

When the result is displayed at the bottom left part of the screen, select the button or the FILE / SAVE RESULT menu and enter a file name.

The text displayed in the Information field will be automatically saved with the chromatogram. The text corresponds to the description of the calculation which was processed to obtain the chromatogram. If a user wants to add more information, this is entered in the Additional information field.



The defined information will be displayed in CompassCDS at the chromatogram opening, in the Open / Save file box, and in the chromatogram properties.

Loading a Virtual Chromatogram in CompassCDS

After the calculation, the chromatogram displayed in the Result section can then be exported into CompassCDS.

Users can choose to either export the generated chromatogram while the Plug-in remains open:

Select the FILE/ OPEN RESULT IN COMPASSCDS menu or click on the button.

Or to export the generated chromatogram and automatically close the Plug-in:

Select the FILE/ GOING BACK TO COMPASSCDS WITH RESULTS menu or click on the button.

In both cases, the export chromatogram default name is ArithmeticChromatogram.VIRT.

NOTE: Once an exported chromatogram is open in CompassCDS, no other chromatogram can be exported from the Plug-in unless the first chromatogram is closed.

Returning to CompassCDS without Generating a Virtual Chromatogram

Select the button, or the FILE / CLOSE menu to come back to CompassCDS without any results.

The Plug-in is automatically closed.